MATHEMATICAL COUPLING OF DISPERATE SPATIAL AND TEMPORAL SCALES IN MULTIPHASE SYSTEMS

ABSTRACT:

In this presentation, we report on new hybrid mathematical algorithms to couple spatial and temporal scales self consistently from molecular to macroscopic/continuum mechanics. These new algorithms will be used in a mathematical tool that will be developed to analyze large multiphase systems of particles (or droplets) dispersed in a fluid. In this class of problems, there are large areas where classical continuum modeling holds. However the nonlinearities and the irreversibilities that can dominate the macroscopic behavior are the result of atomistic scale interactions in the thin films that separate the particles. Insights gained from the detailed calculations of the interaction of a few particles will be rigorously tested and will form the basis of an expert system approach to address larger problems in a computationally tractable manner.

During most of the last century, much of the research activity in multiphase flows was devoted to the solution of the continuum-level Navier-Stokes equations. Only a handful of exact analytical solutions were discovered, and it was impossible to distinguish real physical insights from artifacts of numerical inaccuracies. More recently, new mathematical algorithms based on combination of theory and numerical modeling have allow solutions of the complex macroscopic conservation equations. We know now that even highly precise solutions of the macroscopic conservation equations cannot predict experimentally observed behavior of these systems and do not even scale correctly with the size of the particles. Addition of artificial constants or repulsive forces can produce closer comparisons with observed phenomena, but there is no first-principle-based understanding of the origins of these corrections and no ability to determine them a priori.

A new set of mathematical tools is required to understand and predict the behavior of these systems. Existing hybrid techniques generally involve a direct transition between the molecular dynamics (MD) and continuum regions and in some cases require artificial techniques to conserve mass and momentum. In this work, the transition is done via intermediate transition regions where potentials, constructed to interact with the molecular dynamics regions, are accordant with the fluctuating continuum solution. This provides for a self-consistent, smooth scale coupling. These potentials are generated from the same potential energy functions as the ones employed in the MD region. Diffuse blobs of molecules are generated or "reverse engineered" from the continuum solutions by a procedure similar to that of smoothed particle hydrodynamics, and the use of fluctuating conservation equations preserves the correct hierarchy of fluctuations.